Supporting Information

Metal–Indolizine Zwitterion Complexes as a New Class of Organometallic Material: a Spectroscopic and Theoretical Investigation

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Supporting Information

Table S1. UV-vis absorption data of **1** and **2** in MeOH and acetone at 298K

complex	λ_{max}/nm (ε_{max}/$dm^3mol^{-1}cm^{-1}$)
	solvent = MeOH
1a	261 (sh, 9700), 294 (sh, 3050), 436 (7900)
1b	283 (sh, 5690), 305 (sh, 4490), 458 (11900)
1c	286 (9950), 332 (sh, 4130), 504 (6280)
2a	253 (sh, 15170), 292 (25830), 410 (9360), 465 (sh, 5340)
2b	292 (26690), 430 (10610), 464 (sh, 9000)
2c	291 (25560), 334 (sh, 6080), 463 (7990)
	solvent = $(CH_3)_2CO$
1a	439 (8400)
1b	468 (8940)
1c	507 (5810)
2a	412 (10160), 464 (sh, 6170)
2b	431 (11940), 464 (sh, 10200)
2c	466 (9700)

Table S2. Cartesian coordinates of **1a** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
C	12.534194	6.471648	1.838495
C	13.346331	5.429814	2.144916
H	13.745364	5.086807	3.093403
N	13.715137	4.670868	0.995261
C	12.370692	6.442496	0.305000
C	13.021610	7.660010	-0.350764
H	12.505499	8.568292	-0.030584
H	12.957350	7.581161	-1.444286
H	14.077252	7.741874	-0.070160
C	14.501154	3.581253	0.955410
C	14.743395	2.966485	-0.263437
C	14.162262	3.482558	-1.421631
H	14.346631	3.005184	-2.382104
C	13.344612	4.615691	-1.342745
H	12.871571	5.036350	-2.227488
C	10.106123	9.580143	5.407302
C	9.372929	10.383019	6.360997
H	8.756416	9.740191	6.999302
H	8.721564	11.082215	5.822735
H	10.066569	10.951972	6.989893
C	9.912579	10.387539	1.982302
H	9.174483	10.781119	1.274757
H	9.483660	10.441865	2.986049
C	11.198725	11.207087	1.863705
H	11.637925	11.071901	0.863709
H	10.891039	12.260872	1.904609
C	12.284001	11.041616	2.929196
H	11.871875	11.097828	3.941112
H	13.025904	11.839278	2.810720
C	14.317610	9.400407	4.185009
H	15.217832	8.900150	3.809505
H	14.599340	10.425210	4.452076
C	13.748115	8.669169	5.383425
H	12.935751	9.229084	5.857099
H	14.538066	8.499622	6.124694
C	12.120496	6.516409	6.299103
H	12.844362	6.140006	7.030273
H	11.622723	7.393761	6.727886
C	11.114773	5.419629	5.953512
H	11.596235	4.625929	5.363329
H	10.836843	4.941552	6.902016
C	9.809580	5.867152	5.296786
H	9.430845	6.786400	5.758208
H	9.047008	5.090114	5.419131
C	8.480303	7.132026	3.141740
H	7.612598	6.461275	3.158558
H	8.363939	7.874315	3.937750
C	8.608634	7.784800	1.778804
H	7.796397	8.500398	1.607044
H	8.573757	7.035595	0.979967
C	13.144757	5.200846	-0.110196
N	10.669358	8.955846	4.610607
O	11.015300	6.316188	-0.051588
H	10.848372	6.826102	-0.850595
Ru	11.632952	7.762274	3.148200
S	10.204490	8.651692	1.489767
S	13.201293	9.469376	2.723568
S	13.094551	7.043232	4.845642
S	9.982763	6.135307	3.498476
H	15.379042	2.085142	-0.295245
H	14.913329	3.231240	1.898326

Table S3. Cartesian coordinates of **1b** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
C	12.515174	6.453815	1.841077
C	13.346318	5.424785	2.158687
H	13.728083	5.081548	3.114140
N	13.776519	4.701592	1.013672
C	12.378165	6.430416	0.307053
C	12.956956	7.672789	-0.366487
H	12.352812	8.544462	-0.106277
H	12.944986	7.537422	-1.455590
H	13.990744	7.851473	-0.050205
C	14.600704	3.644509	0.933640
C	14.870096	3.126878	-0.323854
C	14.268730	3.729959	-1.426546
H	14.454967	3.354228	-2.432551
C	10.146100	9.598561	5.416548
C	9.492564	10.431390	6.401088
H	8.879144	9.814922	7.067903
H	8.848887	11.159519	5.892919
H	10.239192	10.968696	6.996645
C	9.926698	10.376195	1.959976
H	9.194149	10.779647	1.252336
H	9.500362	10.439715	2.964492
C	11.225283	11.175736	1.837358
H	11.667831	11.022121	0.841607
H	10.932909	12.234235	1.863536
C	12.302949	11.008079	2.910288
H	11.888074	11.083537	3.919711
H	13.058239	11.792085	2.785438
C	14.306502	9.337650	4.186168
H	15.198739	8.821874	3.812664
H	14.604800	10.358630	4.449766
C	13.726684	8.620053	5.387844
H	12.928910	9.197109	5.865337
H	14.516189	8.434975	6.125837
C	12.056991	6.501136	6.311104
H	12.775168	6.115356	7.043079
H	11.573932	7.387285	6.738173
C	11.034151	5.419571	5.968536
H	11.504385	4.613275	5.386625
H	10.743589	4.953670	6.919279
C	9.740226	5.885369	5.302470
H	9.375900	6.815141	5.754344
H	8.963339	5.123221	5.428072
C	8.439654	7.157156	3.139267
H	7.558749	6.504238	3.165849
H	8.342223	7.909131	3.928962
C	8.576924	7.795595	1.770676
H	7.777141	8.523980	1.594266
H	8.527449	7.041619	0.976922
C	13.227427	5.238962	-0.105587
N	10.657595	8.954553	4.601116
O	11.033707	6.202639	-0.039452
H	10.905592	6.436963	-0.965637
Ru	11.595627	7.737749	3.145432
S	10.186909	8.632293	1.474319
S	13.193354	9.419870	2.722417
S	13.039581	7.006322	4.856564
S	9.922951	6.135108	3.502357
H	15.531242	2.271795	-0.435659
H	15.015944	3.252222	1.858814
N	13.449747	4.787163	-1.307477

Table S4. Cartesian coordinates of **1c** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
C	12.564347	6.504692	1.855035
C	13.413377	5.492290	2.158642
H	13.814061	5.187420	3.116085
N	13.837290	4.764094	1.001083
C	12.430245	6.482595	0.320467
C	13.023795	7.735495	-0.324349
H	12.437519	8.609158	-0.029448
H	12.999484	7.647163	-1.418436
H	14.061988	7.889992	-0.011451
C	14.686803	3.682716	0.955832
C	15.015326	3.155829	-0.328720
C	14.423155	3.725655	-1.481088
H	14.673031	3.315336	-2.458567
C	13.539906	4.780466	-1.363374
H	13.058249	5.223965	-2.231853
C	15.218544	3.097341	2.122672
H	14.943960	3.471193	3.104865
C	16.081980	2.027257	2.007522
H	16.488689	1.569797	2.907687
C	16.444260	1.512012	0.742348
H	17.130567	0.669393	0.678071
C	15.917138	2.063134	-0.402434
H	16.177861	1.664794	-1.382026
C	10.101691	9.610755	5.406713
C	9.386925	10.431407	6.358970
H	8.763471	9.802301	7.004094
H	8.744745	11.138787	5.820463
H	10.093504	10.992144	6.980888
C	9.820448	10.319443	1.954187
H	9.062683	10.674536	1.247303
H	9.406351	10.391031	2.963174
C	11.085535	11.164291	1.791046
H	11.517377	11.001699	0.791809
H	10.754745	12.211738	1.794764
C	12.185341	11.062399	2.850387
H	11.781387	11.139872	3.864097
H	12.904825	11.874754	2.699274
C	14.279010	9.503150	4.126570
H	15.187493	9.021172	3.746851
H	14.535259	10.540771	4.368988
C	13.748984	8.780636	5.347579
H	12.929968	9.328154	5.824118
H	14.555316	8.646203	6.078522
C	12.194697	6.601598	6.333773
H	12.940888	6.253724	7.056443
H	11.684583	7.474142	6.758008
C	11.209396	5.476162	6.025408
H	11.698899	4.683311	5.440438
H	10.960252	5.008414	6.987033
C	9.883126	5.880776	5.383329
H	9.493602	6.802940	5.829758
H	9.139562	5.091165	5.536528
C	8.487575	7.057679	3.215254
H	7.638365	6.364986	3.260751
H	8.361622	7.817731	3.992977
C	8.583350	7.677450	1.834365
H	7.750179	8.365904	1.652279
H	8.560007	6.907122	1.055059
C	13.281386	5.292138	-0.093234

N	10.652888	8.971747	4.613314
O	11.093137	6.274425	-0.065292
H	10.899755	6.804092	-0.845318
Ru	11.621901	7.771377	3.167415
S	10.150601	8.579710	1.505749
S	13.140342	9.509094	2.681228
S	13.128550	7.126561	4.853229
S	10.021301	6.109917	3.576548

Table S5. Cartesian coordinates of **2a** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
H	-0.605962	-2.446067	1.875438
C	-1.110220	-2.041291	1.003239
C	-0.746892	-1.078919	0.119722
C	-1.929230	-0.928534	-0.854319
C	-2.850328	-2.074557	-0.466603
N	-2.358730	-2.640847	0.660508
C	-2.981691	-3.646167	1.299340
H	-2.512465	-4.025431	2.203403
C	-4.159475	-4.152617	0.773023
H	-4.658795	-4.970375	1.286516
C	-4.679871	-3.608189	-0.401464
H	-5.595499	-4.010055	-0.830019
C	-4.017696	-2.546378	-1.028005
H	-4.400952	-2.094773	-1.940057
C	-2.694084	0.372621	-0.591640
O	-1.586407	-0.935912	-2.213613
H	-1.074374	-1.726554	-2.410943
Ru	1.036247	-0.066374	0.041536
N	0.350291	1.625269	-0.982350
C	0.231744	1.754147	-2.311807
H	0.290326	0.837348	-2.892799
C	0.023591	2.981956	-2.928177
H	-0.064230	3.031368	-4.011330
C	-0.065960	4.125795	-2.138053
H	-0.212662	5.105291	-2.589359
C	0.015905	3.991372	-0.757018
H	-0.073600	4.865602	-0.117924
C	0.211806	2.725290	-0.200363
C	0.236463	2.467326	1.246717
C	-0.002860	3.447077	2.212276
H	-0.170887	4.479791	1.918435
C	-0.037616	3.089584	3.554921
H	-0.215407	3.843621	4.318810
C	0.137802	1.750996	3.899084
H	0.092381	1.414710	4.932675
C	0.381376	0.829838	2.889852
H	0.523053	-0.223837	3.122594
N	0.462639	1.179318	1.598525
S	3.243216	0.953088	-0.038752
C	3.753355	0.551637	-1.746370
H	3.202937	1.268786	-2.366445
H	4.820550	0.777985	-1.857779
C	3.463909	-0.874638	-2.153002
H	3.639368	-1.007307	-3.226512
H	4.110363	-1.583874	-1.626153
S	1.710304	-1.331172	-1.817320
C	1.927913	-3.004469	-1.119385
H	0.908689	-3.398501	-1.039277
H	2.465192	-3.616733	-1.852372
C	2.635043	-3.026830	0.216386
H	2.480442	-3.993218	0.708829
H	3.715009	-2.880126	0.109393
S	1.997811	-1.734962	1.369118
C	3.531813	-0.953319	1.978811
H	3.181969	-0.301261	2.788291
H	4.157593	-1.729113	2.435863
C	4.314705	-0.173021	0.946462
H	5.066068	0.447387	1.447883
H	4.846530	-0.832364	0.252298

H	-2.042184	1.223435	-0.795396
H	-3.562204	0.426098	-1.257715
H	-3.038673	0.428359	0.446198

Table S6. Cartesian coordinates of **2b** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
H	-0.602640	-2.430962	1.899538
C	-1.107825	-2.044461	1.019549
C	-0.745118	-1.093476	0.117804
C	-1.919259	-0.970354	-0.869543
C	-2.844762	-2.104234	-0.456528
N	-2.351094	-2.647374	0.688531
C	-3.013586	-3.626219	1.326023
H	-2.582693	-4.015610	2.245285
C	-4.194171	-4.080832	0.761856
H	-4.759056	-4.875168	1.242066
C	-4.629219	-3.489692	-0.423418
H	-5.547793	-3.823413	-0.904755
C	-2.714945	0.320032	-0.650072
O	-1.567376	-1.012923	-2.222854
H	-1.062122	-1.811874	-2.402601
Ru	1.032054	-0.078666	0.045368
N	0.330647	1.610051	-0.973754
C	0.199107	1.737085	-2.302203
H	0.258681	0.820079	-2.883065
C	-0.023172	2.963085	-2.917286
H	-0.122405	3.011086	-3.999454
C	-0.112170	4.106843	-2.127051
H	-0.270064	5.084982	-2.577484
C	-0.015197	3.974172	-0.746818
H	-0.103590	4.848556	-0.107780
C	0.194134	2.709736	-0.191244
C	0.238724	2.454796	1.256167
C	0.020464	3.438148	2.222936
H	-0.146533	4.471142	1.929478
C	0.008171	3.084619	3.567100
H	-0.151401	3.841995	4.331767
C	0.183265	1.746314	3.912013
H	0.155471	1.413264	4.947290
C	0.405221	0.821402	2.901169
H	0.547531	-0.231936	3.135093
N	0.466126	1.166906	1.607774
S	3.232514	0.959923	-0.030177
C	3.746892	0.567279	-1.738261
H	3.190508	1.280728	-2.357223
H	4.812073	0.803561	-1.848399
C	3.470937	-0.860705	-2.147293
H	3.650195	-0.990393	-3.220522
H	4.122056	-1.565166	-1.619875
S	1.720406	-1.332380	-1.818097
C	1.950128	-3.004846	-1.121945
H	0.933983	-3.406918	-1.042071
H	2.491425	-3.612586	-1.855702
C	2.658345	-3.023728	0.213170
H	2.514588	-3.993078	0.702962
H	3.736624	-2.865433	0.105620
S	2.008968	-1.742005	1.369731
C	3.535950	-0.948444	1.982770
H	3.180596	-0.301499	2.793943
H	4.167667	-1.720421	2.438039
C	4.312886	-0.159022	0.953001
H	5.058266	0.466861	1.456630
H	4.851376	-0.811832	0.257840
H	-2.089844	1.176638	-0.906557
H	-3.592492	0.306249	-1.305119

H	-3.045646	0.416684	0.389319
N	-3.953711	-2.494569	-1.018983

Table S7. Cartesian coordinates of **2c** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
H	-0.575726	-2.355920	1.883292
C	-1.091244	-2.002085	0.998782
C	-0.705852	-1.093129	0.069521
C	-1.879399	-0.992766	-0.918809
C	-2.809981	-2.108079	-0.473479
N	-2.348524	-2.604342	0.680650
C	-4.675419	-3.589466	-0.410230
H	-5.584053	-4.002636	-0.844947
C	-3.980591	-2.586704	-1.057295
H	-4.316659	-2.171961	-2.004370
C	-2.654877	0.316849	-0.726847
O	-1.536157	-1.068288	-2.274805
H	-1.036684	-1.874932	-2.435224
Ru	1.082457	-0.079645	0.002611
N	0.379527	1.631155	-0.979569
C	0.289073	1.804405	-2.306585
H	0.395252	0.912248	-2.919195
C	0.056728	3.046312	-2.885398
H	-0.005339	3.132094	-3.968098
C	-0.087417	4.157807	-2.058116
H	-0.252989	5.148140	-2.478222
C	-0.035525	3.975848	-0.681233
H	-0.167162	4.823381	-0.014154
C	0.186309	2.697296	-0.164152
C	0.179936	2.390505	1.273425
C	-0.155541	3.322994	2.257203
H	-0.378532	4.351609	1.986821
C	-0.224324	2.920851	3.585830
H	-0.483169	3.636380	4.363253
C	0.023400	1.585865	3.896411
H	-0.042157	1.213748	4.916540
C	0.362585	0.714188	2.870300
H	0.562128	-0.334564	3.079531
N	0.465995	1.106105	1.592985
S	3.278990	0.958143	-0.033110
C	3.805672	0.603048	-1.746700
H	3.256680	1.332215	-2.353725
H	4.872662	0.837227	-1.842805
C	3.527437	-0.814842	-2.188696
H	3.720636	-0.924018	-3.261732
H	4.168032	-1.532843	-1.666700
S	1.769629	-1.280461	-1.891443
C	1.978293	-2.974589	-1.244262
H	0.957230	-3.366913	-1.178807
H	2.515206	-3.568516	-1.992388
C	2.681297	-3.039185	0.092480
H	2.522688	-4.019510	0.555350
H	3.761941	-2.891955	-0.006453
S	2.042823	-1.780875	1.281251
C	3.569288	-1.012148	1.925697
H	3.208659	-0.392213	2.755545
H	4.197831	-1.799077	2.359068
C	4.351967	-0.188795	0.926664
H	5.091623	0.422618	1.455597
H	4.897330	-0.819819	0.216984
H	-2.009916	1.156467	-0.989684
H	-3.527776	0.324017	-1.388671
H	-2.991877	0.434539	0.308257
C	-3.014462	-3.573738	1.393998

C	-4.215253	-4.096794	0.828774
C	-2.538897	-4.052142	2.631589
H	-1.637868	-3.642555	3.078310
C	-3.242097	-5.041815	3.286375
H	-2.872792	-5.415432	4.239619
C	-4.428307	-5.579642	2.737877
H	-4.965739	-6.358175	3.276252
C	-4.909281	-5.111648	1.536985
H	-5.825344	-5.513719	1.108086

Table S8. Cartesian coordinates of **2a*** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
Ru	-0.020209	-0.120816	-0.011046
C	0.044016	-0.058733	2.031914
C	1.085155	-0.221038	2.874754
H	2.142356	-0.388496	2.691798
C	-1.198261	0.239472	2.904066
C	-0.663747	0.034717	4.309803
N	0.670784	-0.162159	4.241107
C	1.441388	-0.300111	5.333147
H	2.507759	-0.442489	5.175317
C	0.844206	-0.269577	6.583112
H	1.463771	-0.386974	7.468234
C	-0.537859	-0.103933	6.685100
H	-1.017059	-0.094420	7.662434
C	-1.306658	0.055051	5.528745
H	-2.384391	0.197532	5.572093
C	-1.613340	1.707087	2.785102
O	-2.323778	-0.544560	2.646051
H	-2.103667	-1.475128	2.762733
N	-1.860734	0.632527	-0.433487
C	-3.037565	-0.044977	-0.424499
H	-2.979919	-1.108723	-0.203405
C	-4.249246	0.549138	-0.666843
H	-5.157950	-0.047218	-0.651597
C	-4.275245	1.948996	-0.936295
H	-5.218066	2.455601	-1.135051
C	-3.099263	2.657591	-0.937028
H	-3.108434	3.728645	-1.126809
C	-1.864982	2.011773	-0.674112
C	-0.613571	2.675630	-0.551323
C	-0.400242	4.061932	-0.771832
H	-1.222428	4.683212	-1.118724
C	0.840215	4.614762	-0.550673
H	1.006806	5.675621	-0.730210
C	1.893770	3.796631	-0.083921
H	2.881321	4.197205	0.130108
C	1.637268	2.452747	0.106750
H	2.418529	1.790643	0.478418
N	0.442153	1.892041	-0.137395
S	0.207253	-0.305825	-2.527088
C	-0.822961	-1.789072	-2.771585
H	-1.848852	-1.404994	-2.719360
H	-0.666066	-2.150291	-3.795360
C	-0.591737	-2.922087	-1.797667
H	-1.369150	-3.681548	-1.935201
H	0.369780	-3.413962	-1.973277
S	-0.642591	-2.420892	-0.024516
C	0.862633	-3.233706	0.607284
H	0.835813	-3.045895	1.687191
H	0.753881	-4.314220	0.455814
C	2.147293	-2.739157	-0.017948
H	3.006650	-3.106124	0.553081
H	2.266696	-3.088822	-1.048114
S	2.249780	-0.907616	-0.018123
C	2.850045	-0.540545	-1.699250
H	3.028901	0.540572	-1.690106
H	3.822275	-1.032553	-1.820174
C	1.900831	-0.944100	-2.804359
H	2.256530	-0.527631	-3.753569
H	1.845962	-2.030848	-2.924082

H	-1.969787	1.912777	1.773882
H	-2.426081	1.908582	3.491085
H	-0.774292	2.373190	3.009838

Table S9. Cartesian coordinates of **2b*** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
H	-0.568706	-2.423986	1.835642
C	-1.119106	-2.068223	0.966678
C	-0.765130	-1.069370	0.059418
C	-1.948896	-0.948681	-0.925719
C	-2.840664	-2.109226	-0.500678
N	-2.315284	-2.654447	0.687549
C	-2.978062	-3.709284	1.318876
H	-2.539223	-4.095025	2.234450
C	-4.117242	-4.167179	0.729617
H	-4.668520	-4.983796	1.190261
C	-4.582458	-3.574159	-0.478660
H	-5.484629	-3.929748	-0.970489
C	-2.752337	0.343102	-0.770633
O	-1.585455	-1.028724	-2.286853
H	-1.248186	-1.910489	-2.473452
Ru	0.975180	-0.078542	0.098636
N	0.298579	1.613117	-0.939561
C	0.145683	1.717757	-2.266242
H	0.171368	0.789710	-2.832457
C	-0.070216	2.938998	-2.894475
H	-0.190961	2.972851	-3.974785
C	-0.127404	4.093559	-2.119206
H	-0.280581	5.067267	-2.580595
C	-0.004716	3.981789	-0.738240
H	-0.067728	4.867689	-0.112443
C	0.196806	2.723541	-0.169292
C	0.278179	2.493180	1.282598
C	0.119705	3.499263	2.235368
H	-0.033725	4.530209	1.928481
C	0.151050	3.171380	3.586405
H	0.037191	3.948605	4.339348
C	0.311722	1.838329	3.957358
H	0.316940	1.529335	5.000176
C	0.476291	0.888190	2.960478
H	0.602928	-0.163241	3.210810
N	0.488223	1.209325	1.659834
S	3.240669	0.949909	0.029157
C	3.719801	0.586475	-1.690561
H	3.152313	1.308364	-2.289027
H	4.782106	0.826445	-1.817591
C	3.442271	-0.837229	-2.111758
H	3.628346	-0.957375	-3.185119
H	4.086280	-1.550115	-1.587941
S	1.691937	-1.310763	-1.812247
C	1.899709	-2.982122	-1.115379
H	0.878587	-3.372679	-1.046110
H	2.438086	-3.589581	-1.851589
C	2.607776	-3.020271	0.218929
H	2.464758	-3.999508	0.688860
H	3.686157	-2.862063	0.114111
S	1.970532	-1.767445	1.410905
C	3.500442	-0.978687	2.020586
H	3.151659	-0.327906	2.831272
H	4.120920	-1.757573	2.479263
C	4.293991	-0.201539	0.993622
H	5.052726	0.403371	1.502711
H	4.818747	-0.858635	0.292383
H	-2.170006	1.203198	-1.107841
H	-3.653190	0.262817	-1.389648

H	-3.052688	0.500825	0.270500
N	-3.914448	-2.538993	-1.061991

Table S10. Cartesian coordinates of **2c*** at the PBE0/COSMO optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
H	-0.596317	-2.319418	1.831236
C	-1.149535	-2.006850	0.950065
C	-0.768047	-1.054415	0.002376
C	-1.946927	-0.962489	-0.992325
C	-2.819880	-2.122204	-0.555603
N	-2.340557	-2.604485	0.680594
C	-4.581970	-3.752685	-0.490411
H	-5.447285	-4.226725	-0.947895
C	-3.915031	-2.701032	-1.139384
H	-4.259185	-2.329675	-2.102671
C	-2.725810	0.348457	-0.858505
O	-1.568051	-1.059623	-2.349394
H	-1.235603	-1.947532	-2.516306
Ru	0.976160	-0.091394	0.020247
N	0.320182	1.640545	-0.959558
C	0.210003	1.803674	-2.284544
H	0.247396	0.900219	-2.888829
C	0.033836	3.053275	-2.867443
H	-0.046338	3.135315	-3.949014
C	-0.030240	4.175050	-2.045568
H	-0.148839	5.170341	-2.469695
C	0.043915	4.002651	-0.667571
H	-0.023358	4.862542	-0.006818
C	0.209241	2.718823	-0.145963
C	0.244517	2.427906	1.297439
C	0.043310	3.394061	2.283571
H	-0.110919	4.435055	2.012689
C	0.029719	3.012906	3.620719
H	-0.119955	3.757279	4.400043
C	0.191760	1.667641	3.942491
H	0.163554	1.315800	4.971322
C	0.399386	0.760300	2.913731
H	0.531025	-0.298247	3.128715
N	0.451848	1.131829	1.628157
S	3.228699	0.951639	0.033245
C	3.751713	0.628824	-1.682982
H	3.201106	1.365339	-2.279162
H	4.817678	0.868581	-1.775867
C	3.483282	-0.784658	-2.142776
H	3.703399	-0.884044	-3.211598
H	4.110256	-1.508366	-1.613090
S	1.722810	-1.259753	-1.906742
C	1.914105	-2.954473	-1.261236
H	0.891070	-3.343992	-1.217922
H	2.460528	-3.542789	-2.006884
C	2.602882	-3.036928	0.082068
H	2.445672	-4.027798	0.522539
H	3.683944	-2.883513	-0.000747
S	1.952177	-1.812419	1.294905
C	3.465030	-1.043026	1.967553
H	3.092935	-0.428334	2.796044
H	4.080775	-1.836081	2.407990
C	4.272058	-0.218358	0.988736
H	5.008957	0.378291	1.537956
H	4.823790	-0.845047	0.280373
H	-2.115821	1.193411	-1.185398
H	-3.618521	0.298763	-1.492318
H	-3.040946	0.515264	0.176807
C	-2.998328	-3.607095	1.407255
C	-4.139728	-4.204633	0.800979
C	-2.563343	-4.012033	2.667149

H	-1.710418	-3.533140	3.142722
C	-3.239130	-5.034264	3.342645
H	-2.884141	-5.352937	4.320966
C	-4.354030	-5.639659	2.764050
H	-4.882634	-6.431163	3.292799
C	-4.800791	-5.222686	1.511052
H	-5.674671	-5.689701	1.058994

Table S11. Selected molecular orbital compositions and energies for **1**

		Energy / eV	Ru	Indolizine	[14]aneS4	CH_3CN
1a	HOMO–2	–7.003	62.64	4.55	0.32	32.49
	HOMO–1	–6.196	52.49	10.27	3.64	33.59
	HOMO	–6.056	48.89	25.77	3.56	21.79
	LUMO	–2.357	3.34	93.67	0.74	2.25
	LUMO+1	–1.381	0.71	97.33	0.04	1.92
	LUMO+2	–0.723	27.37	5.22	0.04	67.37
1b	HOMO–2	–7.054	63.07	3.90	0.28	32.75
	HOMO–1	–6.257	52.42	10.12	3.64	33.82
	HOMO	–6.133	49.72	23.60	3.62	23.06
	LUMO	–2.678	3.22	94.10	0.64	2.04
	LUMO+1	–1.885	0.34	98.36	0.04	1.26
	LUMO+2	–0.766	27.25	5.38	0.03	67.34
1c	HOMO–2	–7.005	60.76	6.71	0.38	32.15
	HOMO–1	–6.197	52.92	9.97	3.82	33.29
	HOMO	–6.030	46.66	29.37	3.38	20.58
	LUMO	–2.829	2.40	95.89	0.37	1.35
	LUMO+1	–1.414	0.26	98.54	0.02	1.18
	LUMO+2	–0.812	3.31	82.25	4.65	9.79

Table S12. Selected molecular orbital compositions and energies for **2**

		Energy / eV	Ru	Indolizine	bpy	[9]aneS3
2a	HOMO–2	–6.704	63.93	5.62	8.09	22.35
	HOMO–1	–6.366	57.53	11.12	12.00	19.35
	HOMO	–6.213	46.00	29.11	9.37	15.52
	LUMO	–2.539	3.53	25.06	68.48	2.93
	LUMO+1	–2.411	4.97	72.51	20.26	2.26
	LUMO+2	–1.583	8.01	6.13	80.49	5.38
2b	HOMO–2	–6.761	64.18	5.59	7.97	22.25
	HOMO–1	–6.427	57.85	10.75	11.83	19.56
	HOMO	–6.288	46.24	28.23	9.56	15.97
	LUMO	–2.766	1.79	90.33	6.25	1.63
	LUMO+1	–2.523	6.78	7.31	82.58	3.33
	LUMO+2	–1.963	0.32	98.26	0.54	0.87
2c	HOMO–2	–6.698	62.77	6.15	8.08	23.00
	HOMO–1	–6.382	58.14	10.81	11.54	19.51
	HOMO	–6.189	43.67	33.38	8.51	14.45
	LUMO	–2.898	1.26	95.55	1.96	1.23
	LUMO+1	–2.508	6.42	3.66	86.60	3.31
	LUMO+2	–1.592	7.27	5.77	81.75	5.20

Table S13. Calculated vertical transition energies (λ > 350 nm) for **1** and **2** from the TD-DFT/COSMO Calculations

	λ / nm	Osc. Strength	Contribution
1a	476.109	8.191e-03	79.6% H-1 => LUMO, 18.7% HOMO => LUMO
	435.605	2.677e-01	77.7% HOMO => LUMO, 18.6% H-1 => LUMO
	364.203	6.038e-03	47.4% H-1 => L+2, 42.3% HOMO => L+2, 2.30% H-1 => L+8, 1.44% H-5 => L+2, 1.43% H-2 => LUMO
	352.775	3.824e-03	47.4% HOMO => L+2, 40.2% H-1 => L+2, 3.17% HOMO => L+8, 1.72% H-1 => L+8, 1.70% H-4 => L+2, 1.62% H-3 => L+2
	352.634	1.848e-03	89.0% H-2 => LUMO, 6.24% H-2 => L+2, 1.01% HOMO => L+1
1b	532.987	5.784e-03	73.7% H-1 => LUMO, 24.4% HOMO => LUMO
	464.468	2.947e-01	70.7% HOMO => LUMO, 24.0% H-1 => LUMO, 1.73% HOMO => L+1
	394.182	1.605e-02	88.7% HOMO => L+1, 3.47% H-2 => LUMO, 1.60% HOMO => LUMO, 1.53% H-1 => L+1
	364.428	5.718e-03	42.9% H-1 => L+2, 36.1% HOMO => L+2, 12.8% H-2 => LUMO, 1.74% H-1 => L+8
	350.479	5.798e-03	51.0% HOMO => L+2, 18.4% H-1 => L+2, 17.6% H-2 => LUMO, 4.10% HOMO => L+1, 1.70% HOMO => L+8, 1.37% HOMO => L+7
1c	558.513	1.784e-02	80.2% H-1 => LUMO, 18.2% HOMO => LUMO
	520.115	2.171e-01	79.2% HOMO => LUMO, 18.1% H-1 => LUMO
	371.576	4.392e-03	39.2% H-1 => L+3, 36.5% H-2 => LUMO, 17.2% HOMO => L+3, 1.11% H-1 => L+9
	366.845	4.698e-03	51.2% H-2 => LUMO, 36.5% HOMO => L+3, 5.03% H-1 => L+3, 1.14% HOMO => L+9
	352.629	5.213e-03	43.6% H-1 => L+3, 33.0% HOMO => L+3, 10.2% H-2 => LUMO, 3.39% H-1 => L+9, 2.28% H-3 => L+3, 1.70% HOMO => L+9, 1.02% H-4 => L+3
2a	476.474	6.582e-03	55.8% H-1 => LUMO, 26.6% HOMO => LUMO, 11.8% H-1 => L+1, 3.49% HOMO => L+1
	455.720	1.729e-03	81.2% H-1 => L+1, 14.2% H-1 => LUMO, 2.06% HOMO => L+1
	446.411	1.086e-01	66.2% HOMO => LUMO, 23.8% H-1 => LUMO, 2.97% H-1 => L+1, 2.72% H-2 => LUMO
	419.775	3.429e-02	69.9% H-2 => LUMO, 15.3% H-2 => L+1, 7.18% HOMO => L+1, 2.40% HOMO => LUMO, 1.20% H-2 => L+2
	408.198	1.582e-01	76.0% HOMO => L+1, 9.54% H-2 => L+1, 3.12% H-1 => LUMO, 2.03% H-1 => L+4, 1.67% HOMO => LUMO, 1.31% H-2 => LUMO
	394.792	5.528e-02	65.9% H-2 => L+1, 22.5% H-2 => LUMO, 4.09% HOMO => L+1, 2.27% H-1 => L+5
2b	467.709	6.138e-04	74.2% H-1 => LUMO, 18.0% H-1 => L+1, 4.60% HOMO => L+1, 1.28% HOMO => LUMO

	455.658	4.119e-02	40.0% H-1 => L+1, 27.1% HOMO => LUMO, 18.2% HOMO => L+1, 12.1% H-1 => LUMO
	444.369	1.564e-01	37.4% HOMO => LUMO, 36.1% H-1 => L+1, 14.1% HOMO => L+1, 8.01% H-1 => LUMO
	420.320	6.368e-02	37.8% HOMO => L+1, 24.0% H-2 => LUMO, 17.8% HOMO => LUMO, 14.5% H-2 => L+1, 1.38% H-1 => LUMO, 1.17% H-1 => L+1
	415.778	1.190e-01	70.0% H-2 => LUMO, 10.6% HOMO => L+1, 10.2% HOMO => LUMO, 1.38% H-1 => LUMO, 1.16% HOMO => L+2
	409.781	1.605e-02	78.4% H-2 => L+1, 7.53% HOMO => L+1, 2.06% H-1 => L+5, 1.91% HOMO => LUMO, 1.79% H-1 => L+4, 1.65% H-1 => L+1, 1.62% H-2 => L+3, 1.61% H-2 => LUMO
	383.515	2.614e-02	92.5% HOMO => L+2, 1.52% HOMO => LUMO, 1.12% H-1 => L+2
2c	516.366	8.109e-03	93.6% H-1 => LUMO, 2.26% HOMO => L+1, 1.15% HOMO => LUMO
	492.999	1.998e-01	81.3% HOMO => LUMO, 13.2% HOMO => L+1, 2.76% H-1 => LUMO
	464.749	2.252e-02	75.2% H-1 => L+1, 14.8% HOMO => L+1, 5.61% HOMO => LUMO, 1.42% H-1 => LUMO
	437.752	5.028e-02	58.2% HOMO => L+1, 17.0% H-1 => L+1, 8.53% H-2 => L+1, 6.99% HOMO => LUMO, 4.94% H-2 => LUMO, 1.15% H-1 => L+4
	444.885	3.206e-02	79.8% H-2 => LUMO, 15.0% H-2 => L+1
	417.699	2.314e-02	70.0% H-2 => L+1, 12.1% H-2 => LUMO, 5.63% HOMO => L+1, 3.40% H-1 => L+1, 1.50% HOMO => LUMO, 1.38% H-1 => L+4, 1.17% H-2 => L+2